Amendment to the Claims:

Please amend Claims 1, 3, 4, 13, 14 and 32 as set forth below.

1. (Currently amended) A method for predicting the binding affinity of a peptide for a major histocompatibility (MHC) class I or class II molecule, the method being executed on a computer under the control of a program stored on the computer, comprising the following steps:

a) receiving a representation of a complete or partial three-dimensional structure of a ~~an~~ MHC class I or class II molecule,

b) obtaining an ensemble of conformational representations of peptide backbone structures of said peptide, said conformational representations located within the binding site of said MHC molecule,

c) modeling the side-chains of at least said peptide for each peptide backbone structure of said ensemble in relation to said MHC molecule, ~~at least the side-chains of said peptide,~~ thereby obtaining an ensemble of modeled MHC/peptide complexes, ~~and~~

d) evaluating the binding properties of said peptide for said MHC molecule, comprising at least:

d1) evaluating one or more components of the potential energy of each complex of the ensemble of step c),

d2) evaluating the conformational entropy for the complete ensemble of step c), and

e) outputting said evaluation to a user in a user-readable format.

2. (Original) A method according to claim 1 wherein said representation of step (a) is obtained from one of the following:

- one or more experimentally determined structures obtained by for example X-ray crystallography, nuclear magnetic resonance spectroscopy, scanning microscopy, or
- one or more models derived from an experimentally determined structure, whereby said experimentally determined structure has a high sequence identity to said MHC molecule.

3. (Currently amended) A method according to claim 1 wherein said conformational representation of step (b) is generated by a computer modeling method, said method being able to generate multiple energetically favorable backbone configurations in relation to said MHC molecule.

4. (Currently amended) A method according to claim 1 wherein said conformational representation of step (b) is retrieved from a library of peptide structures pre-oriented in relation to said MHC molecule.

5. (Previously presented) A method according to claim 1 wherein a complex within said ensemble of step (c) is obtained from a side-chain placement algorithm.

6. (Previously presented) A method according to claim 5 wherein the side-chain placement of step (c) not only involves placing the side-chains of the peptide itself, but also involves placing at least one side-chain of said MHC molecule that are in contact with said peptide.

7. (Previously presented) A method according to claim 5 wherein a complex within said ensemble of step (c) is obtained from a side-chain placement algorithm suited for global side-chain optimization.

8. (Previously presented) A method according to claim 5 wherein the side-chain placement algorithm is a dead-end elimination (DEE) algorithm, characterized in that said DEE algorithm eliminates rotameric conformations on the basis of a mathematical criterion that allows the detection of conformations that are not compatible with the globally optimal conformation.

9. (Previously presented) A method according to claim 5 wherein the side-chain placement algorithm is a FASTER algorithm, said algorithm being characterized by a repeated perturbation, relaxation and evaluation step.

10. (Previously presented) A method according to claim 1 wherein the binding affinity of step (d) is represented by a single scoring value for the whole ensemble of MHC/peptide complexes, said scoring value comprising the sum of the conformational entropy for the complete ensemble of MHC/peptide complexes, and the average of the said energetical components of each of the complexes of said ensemble.

11. (Previously presented) A method according to claim 1 wherein the binding affinity of step (d) is evaluated for the global complex, thereby accounting for interactions between pairs of residues from the peptide, the MHC molecule and both the peptide and the MHC molecule.

12. (Previously presented) A method according to claim 1 wherein the entropical component reflects the overall conformational flexibility of the peptide.

13. (Currently amended) A method according to claim 1 wherein the conformational representations of said peptide contained in said library are derived from experimentally determined structures.

14. (Currently amended) A method according to claim 1 wherein the conformational representations of said peptide contained in said library are derived from computer-generated structures.

15. (Previously presented) A method according to claim 1 wherein said peptide comprises one or more non-naturally occurring amino acids.

16-30. (Canceled)

31. (Previously presented) A method according to claim 1 wherein said MHC class I molecule comprises an HLA antigen selected from any of the HLA-A, HLA-B, HLA-C, HLA-E, HLA-F and HLA-G alleles.

32. (Currently amended) A method according to claim[[s]] 1 wherein said MHC class II molecule comprises an HLA antigen selected from any of the HLA-DR, HLA-DQ and HLA-DP gene products.

33-46. (Canceled)